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13. ABSTRACT *(Maximum 200 words)*

This final report describes a program of research investigating quantum effects which become important in ultra-small semiconductor devices, and the manner in which these effects may limit downscaling of individual feature sizes. These structures are important for both dense VLSI and millimeter wave usage. In such small devices, where individual feature sizes may be only a few tens of nanometers, significant device performance is dependent upon dynamic transient response effects which become quantum mechanical in nature. Both the time scale and the space scale involved is such that the quantum nature of the transport can greatly modify the normally expected semiclassical response.

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Final Report

Quantum Transport in Semiconductor Devices

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Quantum Transport in Semiconductor Devices

This final report describes a program of research investigating quantum effects which become important in ultra-small semiconductor devices, and the manner in which these effects may limit downscaling of individual feature sizes. These structures are important for both dense VLSI and millimeter wave usage. In such small devices, where individual feature sizes may be only a few tens of nanometers, significant device performance is dependent upon dynamic transient response effects which become quantum mechanical in nature. Both the time scale and the space scale involved is such that the quantum nature of the transport can greatly modify the normally expected semiclassical response.

A. Introduction

During the last several decades, the growth of large-scale integration has been quite rapid, and expected VHSIC chips will have up to 33 million individual transistors on them. Indeed, the growth of complexity within an individual chip has grown steadily at approximately a factor of 4 for each three year period—e.g., there is a new generation of DRAM introduced each three years, whose complexity increases by a factor of 4. There are, of course, several factors to the growth of complexity, but decreasing feature size is one of the leading factors. As a consequence, it is expected that next year's 16 Mb DRAM will have a 0.5 μm design rule and feature size. Yet, it has been speculated that a limitation will arise near 0.1 μm that will prevent further decreases in feature size.

We can understand the driving forces (and the need for further understanding of the physics) quite easily. In the early 1980's, Hewlett-Packard produced a single-chip microprocessor containing approximately 0.5M devices in its 1 cm^2 area. This chip was

fabricated with essendtially 1.25 μm gate length transistors. Today, we are talking about multi-megabit memories and dense signal processing chips with devices of these same dimensions. Yet, *we are also talking about reaching chip densities of 10^9 devices within a short period of time*. While the first question is what would we use so many devices to accomplish, even if we could reliably fabricate the chips with a meaningful yield, we must also ask just what this does to the required device technology. In general, progress in the integrated circuit field has followed a complicated scaling relationship. This scaling reduces feature sizes by an amount α. To reach a billion transistors, as envisaged, requires a scale-up of a factor of 2000 over the HP chip, which means $\alpha = 4.5$. Thus, if we follow the scaling relationships, we expect to see transistors with gate lengths of only 30 nm! Very few laboratories have produced research devices with gate lengths on this scale and little is understood about the limitations (from the physics) that will determine whether or not these devices are practical. However, it is quite unlikely that the individual transistor size will limit the scaling of ULSI!

What is happening in the reduction of individual feature sizes of a transistor, used as the basic building block for ULSI, is that the critical length (e.g. the gate length or a depletion length) will become so small that it approaches the *coherence length* of the electrons that provide the operation. Over the past several years, it has become evident that this latter length is not the wavelength of the electron itself, but the *inelastic mean free path*, or the length over which the energy coherence is maintained by the electron. With modern modulation doping techniques in heterojunction device structures, this latter length can be more than 1 μm at low temperatures, but there is also evidence that it can be as much as 0.1 μm at room temperature, even in Si. The consequence is that such small devices must now be treated as quantum mechanical objects, and many phenomena become important that have never been treated in the normal classical and semi-classical treatments of semiconductor devices. While this has served

to invigorate studies of quantum behavior in device structures, we are limited in that many of these quantum phenomena are only poorly understood at best.

B. Limits to Ultrasmall Devices

The push in fabricating semiconductor devices is progressively to shrink critical dimensions. As fabrication technology, such as electron-beam lithography, x-ray lithography and the electron-beam-induced resist process, is improved, the critical dimensions of devices can be reduced farther than ever before possible. Simple theory is able to predict how the transconductance will vary as the gate lengths are reduced. In this work, our research group has fabricated a series of ultrasmall MESFETs and HEMTs, with gate lengths in the 0.025–0.08 μm regime, in order to measure transconductance scaling from large devices down to the smallest device size currently fabricated. The question still remaining to be answered is how small can a field-effect transistor be and still operate. We have achieved what may be the first experimental evidence of a fundamental limit to device scaling.

The enhanced DC and microwave characteristics of recently developed MESFETs and AlGaAs/GaAs HEMTs are direct consequences of efforts to decrease the gate length. This improvement of device performance can be explained by the semiconductor device models which are based on the gradual channel approximation. As the gate lengths are reduced further in size, however, the linear dependence of device characteristics with gate length is no longer valid. Device performance of these FETs is dominated by short channel effects and velocity overshoot. Short channel effects are mainly due to a reduced gate aspect ratio. This, in turn, deteriorates device parameters and leads to decreased transconductance and microwave cut-off frequency, and a shifted threshold voltage. On

the other hand, velocity overshoot due to non-stationary electron transport of reduced transit time improves these parameters.

The devices we have made are among the smallest in the world (the Japanese have made such devices with gate lengths as short as 20 nm). From careful studies of the transport properties of these devices, it has been established that they are limited by velocity saturation (Fig. 1) (and concomitant velocity overshoot) and it appears that the current-cutoff mechanism is not simple depletion of the active channel by the gate potential. Rather, it seems that significant current flow is achieved in the smallest devices due to tunneling through the gate-drain potential barrier.

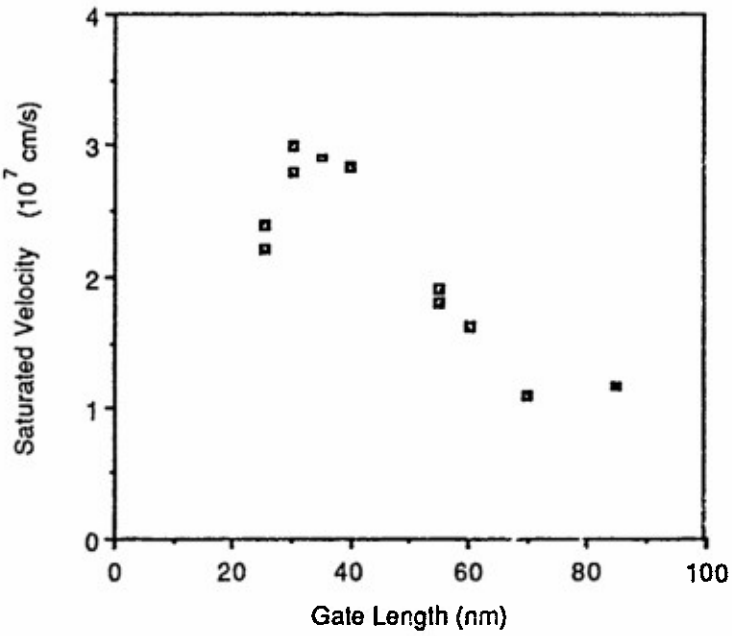

Fig. 1 Saturated velocity measured in ultra-small HEMTs.

The fabrication of both MESFETs and HEMTs with gate lengths in the 25 to 100 nm range has been achieved by electron-beam lithography, on material grown at Ft.

Monmouth (This has been a collaborative effort with P. Newman of that laboratory). Scaling behavior is drawn from experimental data on both transconductance and microwave performance. These devices are essentially velocity saturated devices, so that the only gate length dependence arises from geometrical factors, such as the device aspect ratio, and from transient transport effects. It is found that below 55 to 70 nm, velocity overshoot plays a significant role in device performance. Below 35 nm, the increasing importance of a finite source-drain resistance becomes important, while for the smallest devices (25 nm), the drain-current is thought to be dominated by tunneling of carriers through the depletion potential.

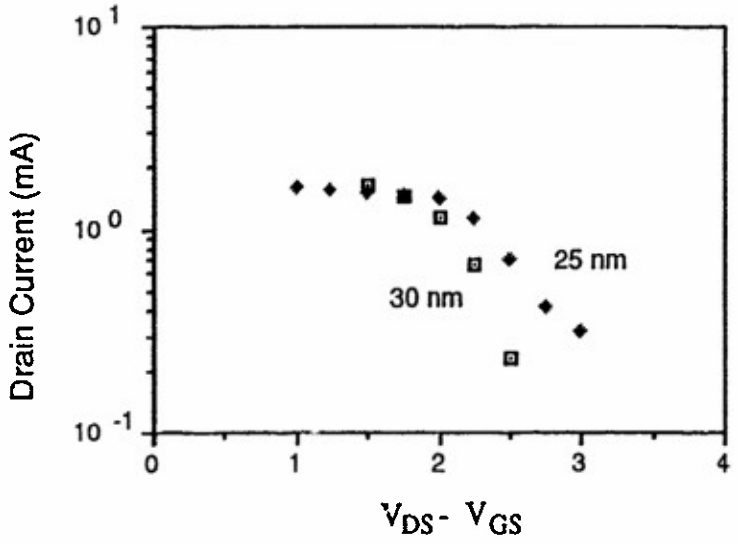

Fig. 2 Behavior of the drain current for the 25 nm devices indicates tunneling by the linear part of the curve.

The devices we have fabricated show the effects of reduced aspect ratios, velocity overshoot, and overshoot saturation. In addition, the HEMTs with gate lengths less than 30 nm indicate that tunneling is occurring in the gate region. This agrees with calculations made from the I-V curves on the other reported sub-30nm gate length device (reported by

scientists from Sony). This tunneling represents the onset of the final scaling limit to FET devices. This is indicated in Fig. 2 by the linear behavior of $\ln(I_{sd})$ with gate-drain potential.

The tunneling limitation is significant for a number of reasons: (1) Prior to the onset of the tunneling mechanism, the transconductance of the devices is continuing to increase with reductions of gate length—only the source resistance limits this rise. (2) If continued improvement in performance is achieved by still smaller sizes, the tunneling current will be strongly (exponentially) dependent upon the *exact* thickness of the barrier region and the barrier potential—hence the current will be exponentially dependent upon fluctuations in the gate length due to the fabrication process. Because of the latter, it may be expected that the current would no longer be a smooth function of the gate voltage, but would show the equivalent of universal conduction fluctuations as various regions along the gate *width* are "turned on" with the gate bias. (3) If small regions of the gate are switched on and off by the bias (tunneling tends to select regions with the lowest barriers, making point emitters), effects such as single electron tunneling can become significant in device operation, even though the devices are not operating at low temperatures.

As mentioned, the rise in transconductance as the gate length is reduced in these devices is attributed to velocity overshoot. The degree to which the velocity can be enhanced by velocity overshoot depends significantly on both the momentum and energy relaxation processes. These devices are heterostructure devices with a significant interface between say the GaAs and the GaAlAs in a normal HEMT. In nearly all current models of transport in these devices, the optical phonons—the interaction that leads to both energy and momentum relaxation—are treated through the bulk modes and bulk interactions. However, it is known that interface modes can exist in these systems, but their effect on

transport has only been investigated briefly. In recent years, these modes have been studied much more intensely, at least theoretically.

C. Modeling of Quantum Effects in MESFETs

As the minimum feature sizes of electronic devices become smaller, velocity overshoot and quantum effects become important. Evidence of these effects has been observed in experimental devices with gates several tens of nanometers long, as discussed above. The accurate modeling of velocity overshoot, in general, requires a treatment which can distinguish momentum and energy relaxation, while tunneling and other phenomena occurring over de Broglie-wavelength scales require a description which incorporates quantum mechanics at some level. We have begun modeling by the quantum moment equations, which satisfies these two requirements.

In principle, large-scale devices can be modeled classically, with an accurate description being given by the Boltzmann transport equation (BTE)

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \Sigma \frac{\partial f}{\partial \mathbf{x}} + e\mathbf{E} \Sigma \frac{\partial f}{\partial \mathbf{p}} = \left. \frac{\partial f}{\partial t} \right|_{coll} . \qquad (1)$$

This equation, however, time-evolves a complete single-particle phase-space distribution $f(\mathbf{x}, \mathbf{p}, t)$. For the simulation of real, three-dimensional devices, this requires prohibitive amounts of memory and computation time. As a practical alternative, one can integrate the BTE with powers of the momentum to derive a set of time-evolution equations for the moments — position-dependent expectation values of powers of the momentum $\langle \mathbf{p}^n \rangle$. This kind of reduced description is useful because a good approximation of the full phase space distribution, as well as most of the quantities of interest, can be determined from the few lowest moments. The hydrodynamic model is based on the first three moment equations, which describe the particle ($n = \langle \mathbf{p}^0 \rangle$), momentum, and energy transport:

$$\frac{\partial n}{\partial t} + \Sigma\left(\frac{\langle p\rangle}{m}\right) = 0\,, \tag{2}$$

$$\frac{\partial \langle p\rangle}{\partial t} + \Sigma\left(\frac{\langle pp\rangle}{m}\right) = -\,nqE - \frac{\langle p\rangle}{\tau_m}\,, \tag{3}$$

$$\frac{\partial \langle p^2\rangle}{\partial t} + \Sigma\left[\frac{\langle p\rangle}{3mn}\left(5\langle p^2\rangle - 2\frac{\langle p\rangle^2}{n}\right)\right] = -\,2qE\Sigma\langle p\rangle - \frac{\langle p^2\rangle - \langle p^2\rangle_0}{\tau_E}\,. \tag{4}$$

Here, the relaxation terms are an approximation to integral terms which involve the scattering cross section. The effective mass m, momentum relaxation time τ_m and energy relaxation time τ_E are all energy dependent and may be obtained from Monte Carlo simulations of bulk material. We have written the equations for a parabolic energy band, and for a purely electrostatic potential. Many simulations of submicron-gate-length semiconductor devices using a hydrodynamic model can be found in the literature. All of these make certain additional approximations whose validity for devices of the sizes now being made must be reexamined.

In general, the moment equations form an infinite hierarchy of equations, corresponding to the fact that an infinite number of moments is needed to recover the information in the complete phase-space distribution. The equations in this hierarchy are coupled to each other by the second term in (1): The time derivative of each moment is related to the gradient of the next higher moment. In order to solve a finite set of equations, one must use some approximate piece of information to "close" the equations. This has been done above by assuming that the momentum distribution is symmetric, in the sense of having a vanishing "skewness". A strong sufficient condition for this is that the distribution depend only on $(p-\langle p\rangle)^2$. In particular, it holds for a drifted-Maxwellian distribution, which has only Gaussian correlations. One physical consequence of this assumption is that heat flow due to the electron gas is not included in the energy equation.

Several groups have succeeded in developing full two-dimensional simulations of semiconductor devices in which the nonequilibrium transport is governed by the

hydrodynamic equations obtained from moments of the Boltzmann transport equation. Our aim is to extend these simulations to include hydrodynamic terms arising from the use of the Wigner equations of motion rather than the Boltzmann equation. The accurate simulation of ultra-small devices requires quantum effects such as tunneling and quantum repulsion (complementary to barrier penetration) to be included. A full quantum description, at the single-particle level, can be based on the Wigner-distribution function f_w, a transform of the density matrix which is a natural generalization of the classical phase-space-distribution function f. This satisfies a time-evolution equation analogous to the BTE which has been successfully used to simulate small quantum devices in one dimension:

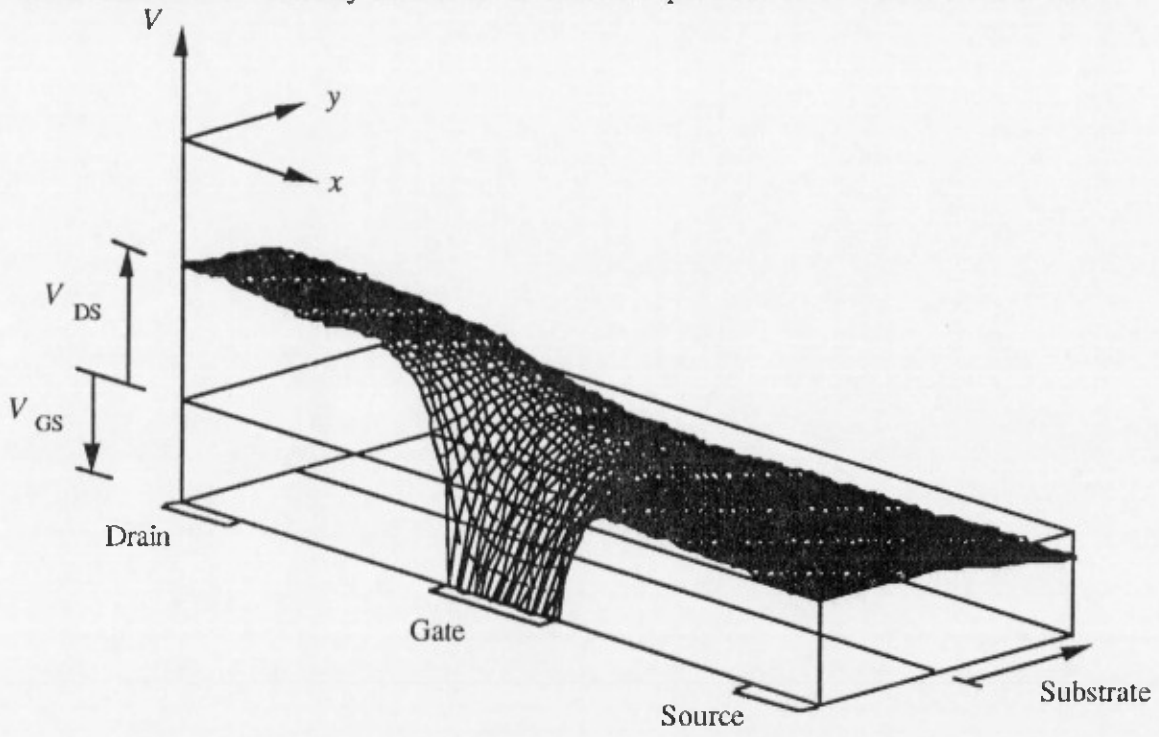

Fig. 3 Potential in a MESFET resulting from solving the hydrodynamic equations simultaneously with Poisson's equation. Here, VGS = – 1.5 V, and VDS = 2 V.

$$\frac{\partial f_W}{\partial t} + \frac{p}{m}\Sigma\nabla f_W + \theta\Sigma f_W = \left.\frac{\partial f_W}{\partial t}\right|_{coll}, \tag{5}$$

where

$$\theta\Sigma f_W = -\frac{2}{\hbar}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}\left(\frac{\hbar}{2}\right)^{2n+1}\frac{\partial^{2n+1}V}{\partial x^{2n+1}}\Sigma\frac{\partial^{2n+1}f_W}{\partial p^{2n+1}}\ . \tag{6}$$

Again, as in the case of the classical equation, the application to higher-dimensional problems imposes a prohibitive computational cost. One is thus led again to a reduced description analogous to the classical hydrodynamic equations derivable from the BTE. In deriving the new equations, one may use the same closure as previously; in particular, a drifted-Fermi-Dirac distribution, like a drifted Maxwellian, has a vanishing skewness, although this is not a sufficient condition, as the stress tensor in (3) must still be separable.

It is a little-remarked fact that the first two quantum-moment equations, computed in this way, are formally identical to the classical hydrodynamic equations, and in particular do not involve $\hbar$. This is not surprising, because their structure reflects particle-number and momentum conservation; if there *were* $O(\hbar)$ corrections, it could imply that the classical conservation laws are only a semiclassical approximation, and fail at long-enough times even in extremely classical situations. The formal equivalence of classical and quantum hydrodynamic equations makes clear that if quantum effects are to be included, then they must already be present in the initial condition for the density distribution. This initial density distribution must be computed by a different method, since the steady-state solution of the moment equations is highly nonunique. In general, of course, one may also include quantum effects by a different closure, in which $\hbar$ appears explicitly, leading to a different generalization of the moment equations. Here, we concentrate on the effects of a proper quantum mechanical initial condition.

However, as pointed out in the early sections, the quantum effects arise from the non-local potential terms, and these contribute a term dependent upon Planck's constant

only in the third moment equation—the energy balance equation. Even here, the term is a small correction which depends upon the gradient of the logarithm of the density, and in a sense leads to the confinement energy of bound states. We can get an idea of what quantum corrections are important by looking at a classical simulation. In Fig. 3, we show the potential in a wide (i.e., two dimensional) short-gate MESFET, obtained by solving the self-consistent hydrodynamic equations (including the energy equation) and Poisson's equation. Here, the gate length is 0.25 μm. In solving equations (2)-(4), a pseudotime approximation was used (in which the convective derivatives are folded into a total "time" partial derivative). The electrostatic potential exhibits sharp structures, which we have previously shown to lead to quantum corrections. In such sharp potential structures, it is necessary to properly account for the initial distribution, which must include the quantum effects. The barrier repulsion, which arises from the quantum nonlocal potentials, is complementary to barrier penetration and tunneling, and it will strongly affect properties near pinchoff, and the bias point at which pinchoff occurs.

If, at the starting point of the simulation, the system is in equilibrium, then the problem of computing a quantum mechanically accurate initial condition is a straightforward one of evaluating common quantum statistical mechanics expressions. In practice this too involves prodigious computation, particularly for high temperatures. At high temperatures, however, the Wigner distribution function must approach the classical one, which has a simple *local* exponential dependence on the potential. Deviations from a local dependence on the potential result essentially from the nonlocalizability of a finite-energy electron. With this motivation, a quasi-classical approximation which explicitly performs the local average of potential over a length scale on the order of the thermal de Broglie wavelength has been adopted. The method is described elsewhere, where we give the parameter values found to optimize the fit to a single semi-infinite barrier at all

temperatures. This fit is shown in Fig. 4, showing excellent agreement with the exact result, which is also shown.

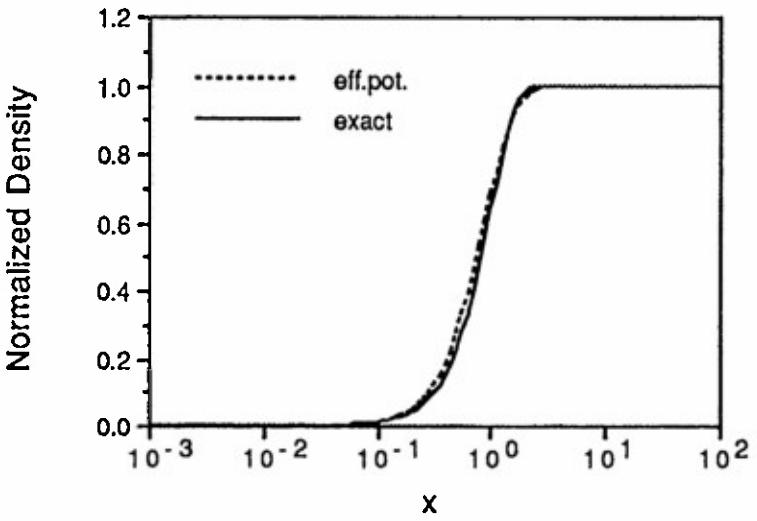

Fig. 4 Comparison of the density arising from the use of an effective potential (for a semi-infinite step in potential) and that from exactly solving the Schrödinger equation.

Using the parameters found for this reference potential, one can test the ability of the approach to reproduce the density in a one-dimensional model of a resonant tunneling diode, for which an exact summation of scattering states *can* be performed rapidly. In Fig. 5, we display a comparison of exact and approximate results, for a double-barrier structure with 50 Å, 0.3 eV barriers, separated by a 50 Å quantum-well region. This computation illustrates two static quantum effects that can be important in short-gate MESFET's. One, the familiar quantum tunneling, is the presence of electrons in the barrier regions, at a density much higher than would follow classically from the fraction in the thermal ensemble having energy above the barrier. The other, complementary effect, follows logically from the continuity of the wavefunction even in potentials with sharp features:

near a barrier, electrons effectively respond to a smeared-out version of the actual potential, having a density reduced relative to the classical density. To apply the effective potential approach to a MESFET configuration requires a more detailed treatment of the boundary condition for the electrostatic potential than is usually done classically. The reason is that the nonlocality of the response to the potential [as can be seen from the preceding discussion or from the third term on the right-hand side of (5)] requires information about the potential in regions that are not classically accessible.

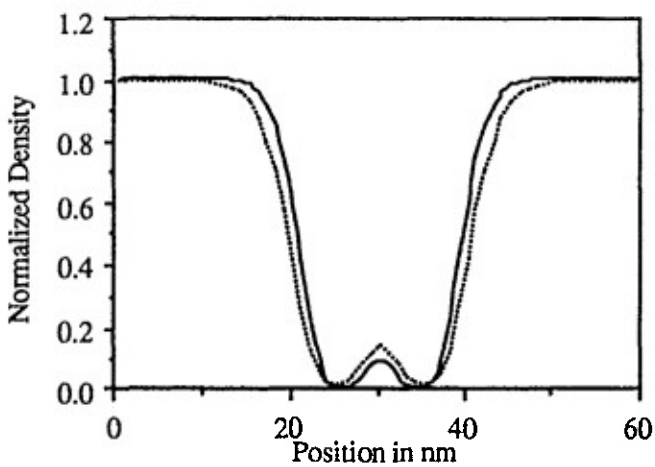

Fig. 5 Electron density computed exactly (sum over scattering states, solid line) and effective potential (broken line).

The goals of the model being developed are to include the statistical potential, and the quantum corrections to the energy equation. These allow us to probe the model of a MESFET (on a lightly doped substrate) to investigate: (1) quantization in the channel well formed between the substrate and the gate potential, (2) tunneling through the gate potential barrier, (3) quantum energy effects on the velocity overshoot, and (4) phase interference effects on the transport in the channel. Although point (1) has been seen experimentally

some years back, it has never been probed in a proper model which included the full dynamics of the carriers. The model here will couple the hydrodynamic equations with an efficient Poisson solver. Two approaches have been investigated: (a) a time-dependent solution technique which iterates between the Poisson solver and the time-step upgraded hydrodynamic equations, and (b) a steady-state solution of the coupled nonlinear set of equations representing the Poisson's and hydrodynamic equations. Much of the numerical algorithm development was carried out in collaboration with Prof. C. Ringhofer, of the Mathematics Department at ASU. This collaboration has been fruitful in previous work on numerical simulations of quantum transport in devices such as the resonant tunneling diode.

D. Publications

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15. J.-R. Zhou and D. K. Ferry, "Simulation of Ultra-Small GaAs MESFETs Using Quantum Moment Equations: II. Velocity Overshoot," submitted for publication.

16. J. R. Zhou and D. K. Ferry, "Simulation of Ultra-Small GaAs HEMTs Using Quantum Moment Equations," in preparation.

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